NAREGI is a collaborative research project between industry, academia, and government organizations. Our goal is to develop a new science grid that will be able to perform large-scale simulations for next-generation R&D.

The Center for Grid Research and Development and the Computational Nano-science Center serve as the bases of project activities. The Center for Grid Research and Development develops grid infrastructure software and network technology. The Computational Nano-science Center evaluates the new grid system using application software and advanced nano-science simulation technology.
R&D-capable computer resources help establish the next-generation industrial infrastructure.
Background of Science Grid R &D (2)

Computing Resource Requirements

- Protein Structure Analysis / Drug Design
- Reaction Condition Optimization / Semiconductor Function Prediction
- Organic Material Function / Reaction Prediction
- Automobile Design / Chip Design

Coupled Simulation Requirements

- Development based on experiment / measurement data
- Development based on combining single-function simulations

Conventional R & D and Product Development

1) Shorter development periods
2) Understanding new phenomena
3) Optimizing designs

Next-generation R & D and Product Development

1) System-wide large-scale analysis
2) Multi-scale analysis
3) Multi-physics analysis

Required computer capacity is based on data from the National Institute of Science and Technology Policy.
NAREGI R&D System

Center for Grid Research and Development
(National Institute of Informatics)

Project Leader (Dr. K. Miura, NII)

Grid Middleware and Upper Layer R&D
Group Leaders

Grid Networking R&D
Group Leaders

MEXT
(Ministry of Education, Culture, Sports, Science and Technology)

National Supercomputing Centers

Coordination in Network Research

SuperSINET

Network Technology Refinement

Coordination Requirements

Computational Nano science Center
(Institute for Molecular Science)

Nano science Applications
Director (Dr. Hirata, IMS)

R&D of Grand-challenge Grid Applications
(ISPP, Tohoku-U, ACAIIT etc.,
Industrial Partners)

ITBL Project (JAIIR)
ITBL Project Dir.

Operations

R&D

Operations

R&D

Utilization of Computing Resources

Consortium for Promotion of Grid Applications in Industry

Grid R&D Advisory Board

Joint Research

Coordination/Deployment

Joint Research

Joint Research

Utilization of Computing Resources

(Titech, Osaka-U, Kyushu-U, etc.)
Relationship among NAREGI Organizations and Outputs of the Project

Center for Grid Research and Development
(National Institute of Informatics)

Grid Middleware
- Resource Management in the Grid Environment
- Grid Programming Environment
- Grid Applications Environment
- High-performance & Secure Grid Networking
- Grid-Enabled Nano-Applications

Science Grid Environment

Evaluation of Grid System with Nano Applications

Computational Nano-science Center
(Institute of Molecular Science)

- Computational Methods for Nano-science using the Latest Grid Technology

Subjects of Research
- Large-scale Computation
- High Throughput Computation
- New Methodology for Computational Science

Vitalization of Industry

- Progress in the Latest Research and Development (Nano, Biotechnology)
- Use in Industry (New Intellectual Product Development)

Consortium for Promotion of Grid Applications in Industry
(Member company: 40 companies)

Requirement from the Industry with regard to Science Grid for Industrial Applications

Solicited Research Proposals from the Industry to Evaluate Grid System with Nano-science Applications

e – Infrastructure

- Productization of General-purpose Grid Middleware for Scientific Computing
- Grid Middleware for Large Computer Centers
- Personnel Training (IT and Application Engineers)
- Contribution to International Scientific Community and Standardization
NAREGI Server Grid

Resource allocation on Server Grid, Automatic scheduling of executing jobs, where users can run their HPC application programs as it is or slightly modified.

Seamless resource coordination across many different research organizations.
NAREGI Middleware Stack

- Grid-Enabled Nano-Applications
  - Grid Visualization
  - Grid PSE
  - Grid Workflow
  - Super Scheduler
  - Distributed Information Service

- (Globus, Condor, UNICORE → OGSA)
  - Grid VM

- Grid Programming
  - Grid RPC
  - Grid MPI

- Packaging

- High-Performance & Secure Grid Networking

- SuperSINET

- Computing Resources
  - NII
  - IMS
  - Research Organizations
  - etc
Scenario for Multi-site MPI Job Execution

1: Submission
2: Negotiation
3: Agreement
4: Reservation
5: Sub-Job
6: Co-Allocation
7: Submission
8: Local Scheduler
9: MPI Server
10: Accounting
11: Monitoring

Input files
Output files
Resource Query
Distributed Information Service
Super Scheduler
Super Scheduler
Super Scheduler

RISM Source
FMO Source
Work-flow

IMPI

GridMPI

GridVM

Site A (SMP machine)
Site B (PC cluster)
Site C (PC cluster)

Scenario for Multi-site MPI Job Execution

National Research Grid Initiative
Adaptation of Nano-science Applications to Grid Environment

MPICH-G2, Globus

Electronic Structure in Solutions

Data Transformation between Different Meshes

Grid Middleware

Solvent Distribution Analysis

Electronic Structure Analysis

Grid Middleware

Reference Interaction Site Model

Fragment Molecular Orbital method
Construction of a Testbed of Heterogeneous Environments for the Verification of Grid System Development

- NAREGI Phase 1 Testbed
- SuperSINET
- TiTech Campus Grid
- Osaka Univ. BioGrid
- Kyoto Univ. Small Test App Clusters
- Kyushu Univ. Small Test App Clusters
- AIST SuperCluster
- AIST Small Test App Clusters
- KEK Small Test App Clusters
- ISSP Small Test App Clusters
- Tohoku Univ. Small Test App Clusters
- Center for GRID R&D (NII) ~5 Tflops
- Computational Nano science Center (IMS) ~10 Tflops
- ~3000 CPUs
- ~17 Tflops
**Computer System for Grid Software Infrastructure R & D**

**Center for Grid Research and Development (5 Tllops, 700GB)**

<table>
<thead>
<tr>
<th>File Server</th>
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<tbody>
<tr>
<td>PRIMEPOWER 900 + ETERNUS3000 + ETERNUS LT160</td>
</tr>
<tr>
<td>1node / 8CPU (SPARC64V1.3GHz)</td>
</tr>
<tr>
<td>Memory 16GB</td>
</tr>
<tr>
<td>Storage 10TB</td>
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<tr>
<td>Back-up Max.36.4TB</td>
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<thead>
<tr>
<th>SMP type Compute Server</th>
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<tbody>
<tr>
<td>(PRIMEPOWER HPC2500)</td>
</tr>
<tr>
<td>1node (UNIX, SPARC64V1.3GHz/64CPU)</td>
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<tr>
<td>Memory 128GB</td>
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<tr>
<td>Storage 441GB</td>
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<tr>
<th>SMP type Compute Server</th>
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<tbody>
<tr>
<td>(SGI Altix3700)</td>
</tr>
<tr>
<td>1node (Itanium2 1.3GHz/32CPU)</td>
</tr>
<tr>
<td>Memory 32GB</td>
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<tr>
<td>Storage 180GB</td>
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<tr>
<th>SMP type Compute Server</th>
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<tbody>
<tr>
<td>(IBM pSeries690)</td>
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<tr>
<td>1node (Power4 1.3GHz/32CPU)</td>
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<tr>
<td>Memory 64GB</td>
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<td>Storage 480GB</td>
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<tr>
<th>Distributed-memory type Compute Server</th>
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<tbody>
<tr>
<td>(PRIMERGY RX200)</td>
</tr>
<tr>
<td>128 CPUs (Xeon, 3.06GHz) + Control Node</td>
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<tr>
<td>Memory 130GB</td>
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<tr>
<td>Storage 9.4TB</td>
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<tr>
<th>Distributed-memory type Compute Server</th>
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<tbody>
<tr>
<td>(Express 5800)</td>
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<tr>
<td>128 CPUs (Xeon, 2.8GHz) + Control Node</td>
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<tr>
<td>Memory 65GB</td>
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<tr>
<td>Storage 4.7TB</td>
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<tr>
<th>Distributed-memory type Compute Server</th>
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<tbody>
<tr>
<td>(HPC LinuxNetworx)</td>
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<tr>
<td>128 CPUs (Xeon, 2.8GHz) + Control Node</td>
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**Intra NW**

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<tr>
<th>L3 SW 1Gbps (upgradable to 10Gbps)</th>
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<tr>
<td>Ext. NW</td>
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<td>Intra NW-A</td>
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<td>Intra NW-B</td>
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**Ext. NW**

| L3 SW 1Gbps (upgradable to 10Gbps) |

**SuperSINET**

**National Research Grid Initiative**
Computer System for Nano Application R & D
Computational Nano science Center (10 TFlops, 5TB)

SMP type Computer Server
5.4 TFLOPS
16ways x 50nodes (POWER4+, 1.7GHz)
Multi-stage Crossbar Network

Distributed-memory type
Computer Server (4 units) 5.0 TFLOPS
818 CPUs (Xeon, 3.06GHz) + Control Nodes
Myrinet 2000 (2Gbps)

File Server
16CPUs (SPARC64 GP, 675MHz)
Memory 8GB
Storage 30TB
Back-up 25TB

Front-end Server
L3 SW
1Gbps
(Upgradable to 10Gbps)

Firewall
CA/RA Server
VPN

SuperSINET

Center for Grid R & D
National Research Grid Initiative
Summary

1) Grid will be not only the information infrastructure, but also the R & D base and the industrial infrastructure in the 21st century.
2) Develop a grid middleware which seamlessly connects heterogeneous computer resources spanned across the nation.
3) Utilize the developed grid infrastructure by conducting research on leading-edge nano science and nano technology simulation applications on top of the infrastructure.
4) Hand down the developed grid technology to industry sector and lead to the strengthening of its international competitiveness.
5) Contribute to international standardization of grid technology